

2,2,3-Trimethylbutane
464-06-2 | DTXSID7060047

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 82.7 °C

Global applicability domain: Inside

Local applicability domain index: 8.88e-01

Confidence level: 9.21e-01

Nearest Neighbors from the Training Set

Image not found

2,2,3-Trimethylbutane

Measured: 80.8

Predicted: 82.7

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2,4-Dimethylpentane

Measured: 80.4

Predicted: 83.6

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Pentane,3,3-dimethyl-

Measured: 86.0

Predicted: 84.5

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Pentane, 2,2-dimethyl-

Measured: 79.2

Predicted: 84.5